



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2025 – 01:11 pm BST

PDB ID : 9RDI / pdb_00009rdi
Title : Crystal Structure of Flap Endonuclease FEN1 with Compound 5
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Deposited on : 2025-06-02
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

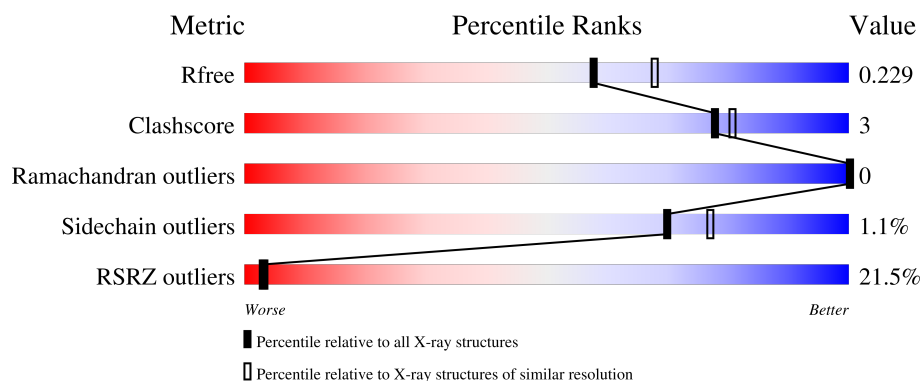
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	342	<div> <div>19%</div> <div>85%</div> <div>5%</div> <div>10%</div> </div>
1	B	342	<div> <div>20%</div> <div>85%</div> <div>7%</div> <div>8%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5332 atoms, of which 30 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

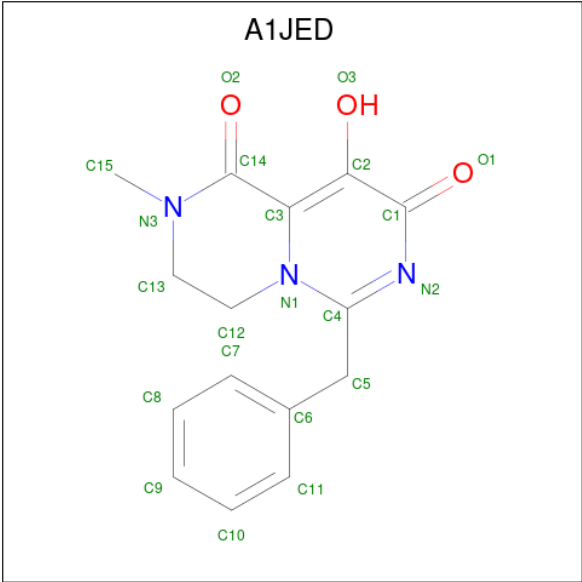
- Molecule 1 is a protein called Flap endonuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2426	1536	418	457	15			
1	B	314	Total	C	N	O	S	0	0	0
			2467	1559	428	465	15			

There are 12 discrepancies between the modelled and reference sequences:

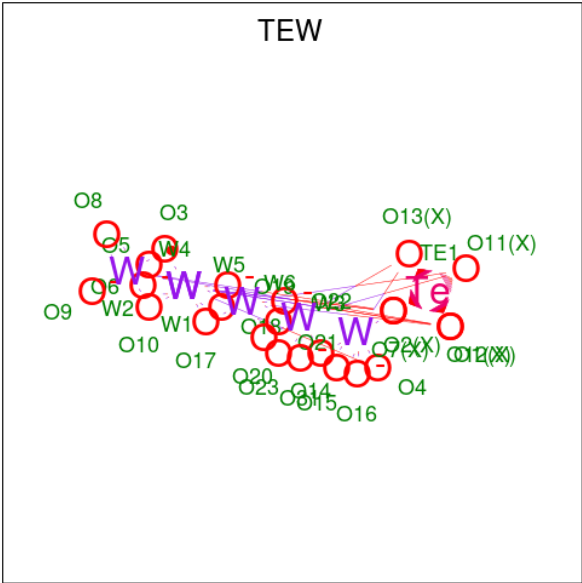
Chain	Residue	Modelled	Actual	Comment	Reference
A	337	LEU	-	expression tag	UNP P39748
A	338	GLU	-	expression tag	UNP P39748
A	339	VAL	-	expression tag	UNP P39748
A	340	LEU	-	expression tag	UNP P39748
A	341	PHE	-	expression tag	UNP P39748
A	342	GLN	-	expression tag	UNP P39748
B	337	LEU	-	expression tag	UNP P39748
B	338	GLU	-	expression tag	UNP P39748
B	339	VAL	-	expression tag	UNP P39748
B	340	LEU	-	expression tag	UNP P39748
B	341	PHE	-	expression tag	UNP P39748
B	342	GLN	-	expression tag	UNP P39748

- Molecule 2 is 2-methyl-9-oxidanyl-6-(phenylmethyl)-3,4-dihydropyrazino[1,2-c]pyrimidine-1,8-dione (CCD ID: A1JED) (formula: C₁₅H₁₅N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	15	0
			36	15	15	3	3		
2	B	1	Total	C	H	N	O	15	0
			36	15	15	3	3		

- Molecule 3 is 6-tungstotellurate(VI) (CCD ID: TEW) (formula: O₂₄TeW₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 31	O 24	Te 1	W 6	0	0
3	A	1	Total 31	O 24	Te 1	W 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 31	O 24	Te 1	W 6	0	0
3	A	1	Total 31	O 24	Te 1	W 6	0	0
3	B	1	Total 31	O 24	Te 1	W 6	0	0
3	B	1	Total 31	O 24	Te 1	W 6	0	0
3	B	1	Total 31	O 24	Te 1	W 6	0	0
3	B	1	Total 62	O 48	Te 2	W 12	0	1
3	B	1	Total 31	O 24	Te 1	W 6	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mg 2	0	0
4	B	2	Total 2	Mg 2	0	0

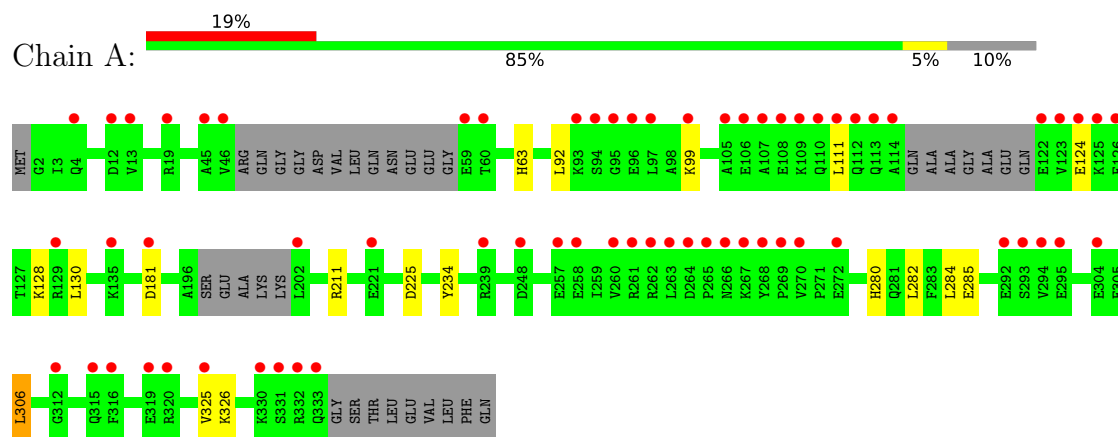
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total 25	O 25	0	0
5	B	28	Total 28	O 28	0	0

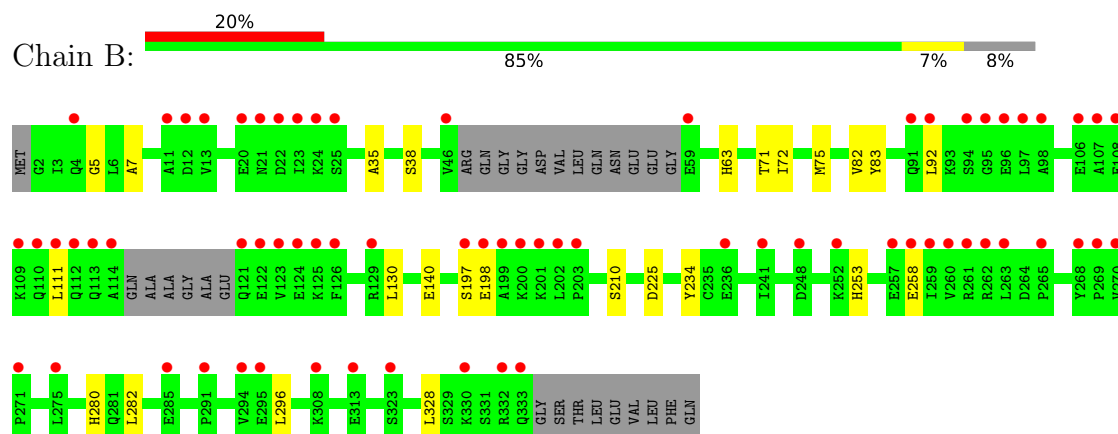
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Flap endonuclease 1



• Molecule 1: Flap endonuclease 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.45Å 116.15Å 139.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.41 – 2.10 40.41 – 2.10	Depositor EDS
% Data completeness (in resolution range)	67.2 (40.41-2.10) 67.2 (40.41-2.10)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.8 (10-JUL-2024)	Depositor
R, R_{free}	0.211 , 0.232 0.203 , 0.229	Depositor DCC
R_{free} test set	1963 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5332	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, A1JED, TEW

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	0/2468	1.07	1/3322 (0.0%)
1	B	0.73	0/2510	1.10	1/3380 (0.0%)
All	All	0.72	0/4978	1.08	2/6702 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	SER	N-CA-C	5.97	118.27	111.11
1	A	181	ASP	CA-CB-CG	5.15	117.75	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2426	0	2422	11	0
1	B	2467	0	2458	16	0
2	A	21	15	0	0	0
2	B	21	15	0	0	0
3	A	124	0	0	2	0
3	B	186	0	0	7	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	25	0	0	0	0
5	B	28	0	0	0	0
All	All	5302	30	4880	27	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:HB2	3:A:405:TEW:O15	1.85	0.76
1:B:5:GLY:HA2	3:B:405[A]:TEW:O8	1.87	0.74
1:A:99:LYS:HE2	3:A:404:TEW:O11	1.89	0.72
1:A:111:LEU:HD22	1:A:130:LEU:HD11	1.79	0.65
1:B:7:ALA:HB3	3:B:405[B]:TEW:O31	1.97	0.63
1:B:5:GLY:HA2	3:B:405[B]:TEW:O23	2.00	0.61
1:B:92:LEU:HD11	1:B:234:TYR:HB3	1.88	0.55
1:B:111:LEU:HD22	1:B:130:LEU:HD11	1.89	0.55
1:A:92:LEU:HD21	1:A:282:LEU:HD22	1.88	0.54
1:B:225:ASP:OD1	1:B:280:HIS:ND1	2.40	0.54
1:B:71:THR:O	1:B:75:MET:HG2	2.07	0.52
1:B:198:GLU:HA	3:B:404:TEW:O8	2.10	0.52
1:B:7:ALA:N	3:B:405[B]:TEW:O31	2.46	0.48
1:B:5:GLY:CA	3:B:405[A]:TEW:O8	2.59	0.47
1:B:72:ILE:HG12	1:B:328:LEU:HB2	1.97	0.45
1:B:7:ALA:CB	3:B:405[B]:TEW:O31	2.62	0.45
1:A:92:LEU:HD11	1:A:234:TYR:HB3	1.99	0.43
1:A:63:HIS:H	1:A:63:HIS:CD2	2.36	0.42
1:B:82:VAL:HG21	1:B:296:LEU:HD22	2.01	0.42
1:A:280:HIS:CD2	1:A:284:LEU:HD12	2.55	0.41
1:B:63:HIS:HE1	1:B:140:GLU:OE1	2.03	0.41
1:A:124:GLU:O	1:A:128:LYS:HG2	2.20	0.41
1:B:35:ALA:HB2	1:B:83:TYR:HB3	2.03	0.41
1:A:225:ASP:OD1	1:A:280:HIS:ND1	2.54	0.41
1:A:306:LEU:HD13	1:A:325:VAL:HG22	2.02	0.41
1:A:280:HIS:NE2	1:A:284:LEU:HD11	2.36	0.40
1:B:253:HIS:HB3	1:B:258:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/342 (88%)	293 (98%)	7 (2%)	0	100	100
1	B	308/342 (90%)	296 (96%)	12 (4%)	0	100	100
All	All	608/684 (89%)	589 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/294 (89%)	259 (99%)	3 (1%)	70	77
1	B	265/294 (90%)	262 (99%)	3 (1%)	70	77
All	All	527/588 (90%)	521 (99%)	6 (1%)	70	77

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	GLU
1	A	306	LEU
1	A	326	LYS
1	B	38	SER
1	B	210	SER
1	B	282	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	63	HIS
1	A	77	ASN
1	A	143	HIS
1	A	273	ASN
1	B	4	GLN
1	B	41	GLN
1	B	63	HIS
1	B	77	ASN
1	B	143	HIS
1	B	253	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TEW	A	403	-	29,42,42	0.99	2 (6%)	12,129,129	4.17	8 (66%)
3	TEW	A	402	-	29,42,42	0.86	1 (3%)	12,129,129	1.47	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TEW	B	403	-	29,42,42	0.80	0	12,129,129	5.75	7 (58%)
3	TEW	B	404	-	29,42,42	1.19	5 (17%)	12,129,129	14.75	10 (83%)
3	TEW	B	406	-	29,42,42	0.94	1 (3%)	12,129,129	1.83	2 (16%)
2	A1JED	A	401	4	23,23,23	0.71	1 (4%)	20,33,33	0.72	0
3	TEW	A	404	-	29,42,42	0.87	1 (3%)	12,129,129	6.05	7 (58%)
3	TEW	A	405	-	29,42,42	0.87	0	12,129,129	0.94	0
2	A1JED	B	401	4	23,23,23	0.97	1 (4%)	20,33,33	0.58	0
3	TEW	B	405[B]	-	29,42,42	0.88	0	12,129,129	2.04	2 (16%)
3	TEW	B	405[A]	-	29,42,42	0.79	0	12,129,129	4.00	6 (50%)
3	TEW	B	402	-	29,42,42	0.85	0	12,129,129	3.32	5 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1JED	A	401	4	-	0/4/17/17	0/3/3/3
2	A1JED	B	401	4	-	0/4/17/17	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	A1JED	C14-N3	3.67	1.40	1.35
3	B	404	TEW	W5-O11	-2.91	2.19	2.34
2	A	401	A1JED	C14-N3	2.54	1.38	1.35
3	A	403	TEW	W3-O2	-2.45	2.21	2.34
3	B	404	TEW	W2-O7	-2.39	2.22	2.34
3	A	403	TEW	W2-O7	-2.38	2.22	2.34
3	A	402	TEW	W2-O7	-2.14	2.23	2.34
3	B	404	TEW	W3-O2	-2.13	2.23	2.34
3	B	404	TEW	W4-O7	-2.09	2.23	2.34
3	B	406	TEW	W5-O11	-2.06	2.23	2.34
3	B	404	TEW	W1-O5	-2.04	1.71	2.10
3	A	404	TEW	W5-O11	-2.02	2.24	2.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	TEW	O1-TE1-O12	34.84	126.01	94.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	TEW	O13-TE1-O12	22.94	115.30	94.65
3	B	404	TEW	O7-TE1-O2	-19.22	77.36	94.65
3	B	404	TEW	O11-TE1-O2	-18.89	77.65	94.65
3	B	403	TEW	O11-TE1-O2	11.16	104.70	94.65
3	A	404	TEW	O1-TE1-O12	10.68	104.27	94.65
3	A	404	TEW	O13-TE1-O1	9.82	103.49	94.65
3	B	404	TEW	O1-TE1-O2	-9.00	74.58	85.21
3	B	403	TEW	O7-TE1-O2	8.49	102.30	94.65
3	A	403	TEW	O7-TE1-O2	-8.22	87.25	94.65
3	A	404	TEW	O11-TE1-O7	-8.00	87.46	94.65
3	B	403	TEW	O13-TE1-O12	-7.89	87.55	94.65
3	B	405[A]	TEW	O13-TE1-O1	7.87	101.74	94.65
3	A	404	TEW	O11-TE1-O2	-7.85	87.58	94.65
3	A	404	TEW	O13-TE1-O12	7.52	101.42	94.65
3	B	402	TEW	O7-TE1-O2	-7.38	88.01	94.65
3	B	405[A]	TEW	O11-TE1-O2	7.26	101.19	94.65
3	A	403	TEW	O1-TE1-O12	7.14	101.08	94.65
3	B	403	TEW	O11-TE1-O7	6.93	100.89	94.65
3	B	403	TEW	O13-TE1-O1	-6.46	88.83	94.65
3	A	403	TEW	O11-TE1-O7	-5.83	89.41	94.65
3	A	404	TEW	O7-TE1-O2	-5.78	89.45	94.65
3	B	405[B]	TEW	O1-TE1-O12	5.66	99.75	94.65
3	B	403	TEW	O1-TE1-O12	-5.66	89.56	94.65
3	B	406	TEW	O13-TE1-O12	-5.09	90.07	94.65
3	B	402	TEW	O13-TE1-O12	4.96	99.12	94.65
3	B	402	TEW	O13-TE1-O1	4.94	99.10	94.65
3	B	404	TEW	O12-TE1-O11	-4.76	79.59	85.21
3	B	405[A]	TEW	O13-TE1-O12	-4.74	90.39	94.65
3	A	403	TEW	O13-TE1-O12	4.45	98.66	94.65
3	B	405[A]	TEW	O11-TE1-O7	-4.36	90.73	94.65
3	B	402	TEW	O11-TE1-O2	3.93	98.19	94.65
3	B	405[A]	TEW	O1-TE1-O12	-3.57	91.44	94.65
3	B	405[A]	TEW	O7-TE1-O2	3.56	97.86	94.65
3	A	403	TEW	O1-TE1-O2	-3.52	81.05	85.21
3	B	404	TEW	O13-TE1-O11	-3.38	81.22	85.21
3	B	404	TEW	O13-TE1-O2	-3.27	81.35	85.21
3	A	402	TEW	O7-TE1-O2	3.22	97.55	94.65
3	B	404	TEW	O7-TE1-O1	-2.97	81.70	85.21
3	A	403	TEW	O13-TE1-O2	2.87	88.60	85.21
3	B	403	TEW	O12-TE1-O11	-2.87	81.82	85.21
3	B	404	TEW	O11-TE1-O7	-2.59	92.33	94.65
3	A	403	TEW	O13-TE1-O1	2.52	96.92	94.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	404	TEW	O13-TE1-O11	-2.46	82.30	85.21
3	A	403	TEW	O12-TE1-O11	-2.35	82.43	85.21
3	A	402	TEW	O11-TE1-O7	-2.31	92.58	94.65
3	B	405[B]	TEW	O12-TE1-O11	-2.31	82.49	85.21
3	B	406	TEW	O7-TE1-O2	2.29	96.71	94.65
3	B	402	TEW	O1-TE1-O12	-2.01	92.84	94.65

There are no chirality outliers.

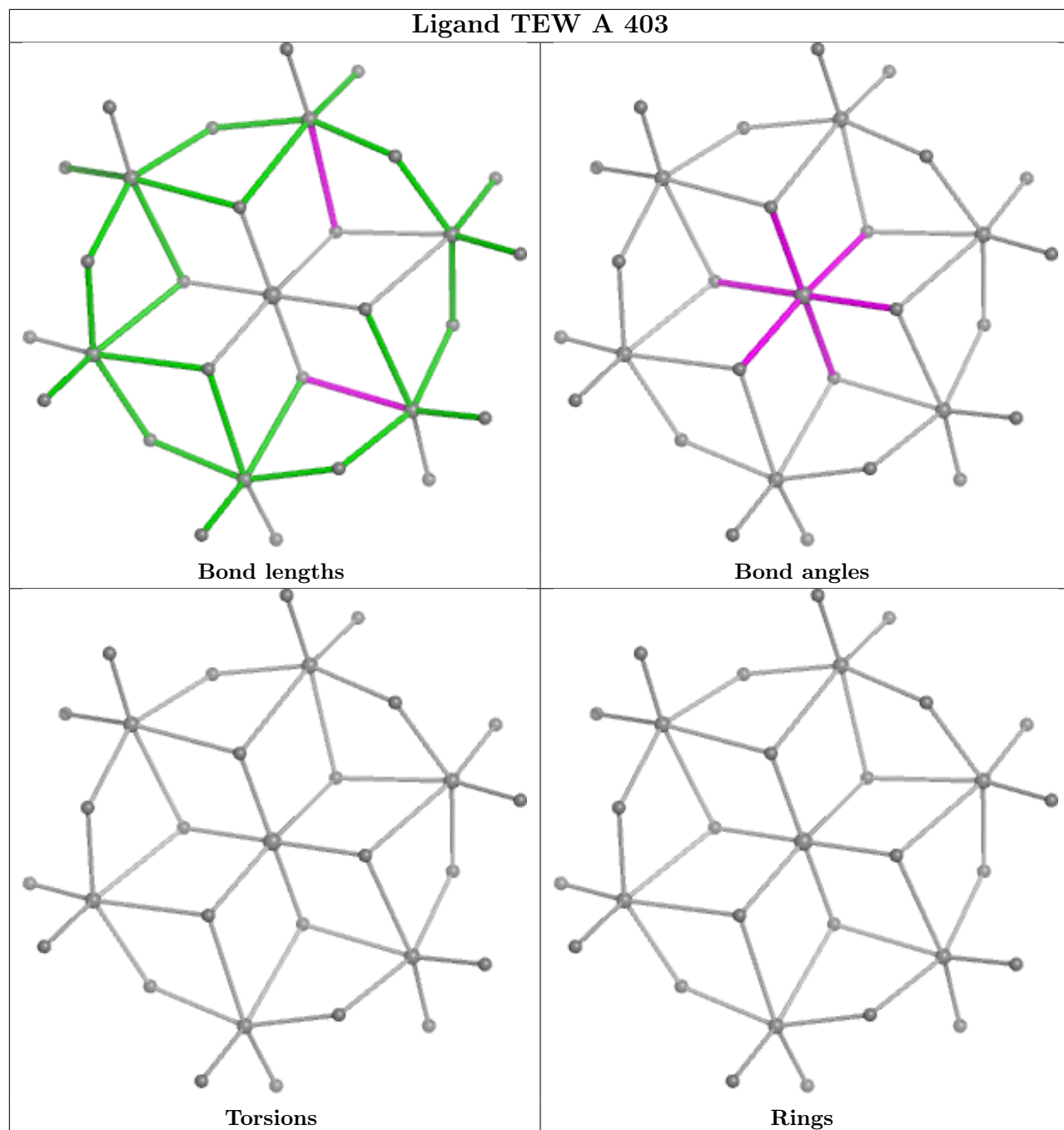
There are no torsion outliers.

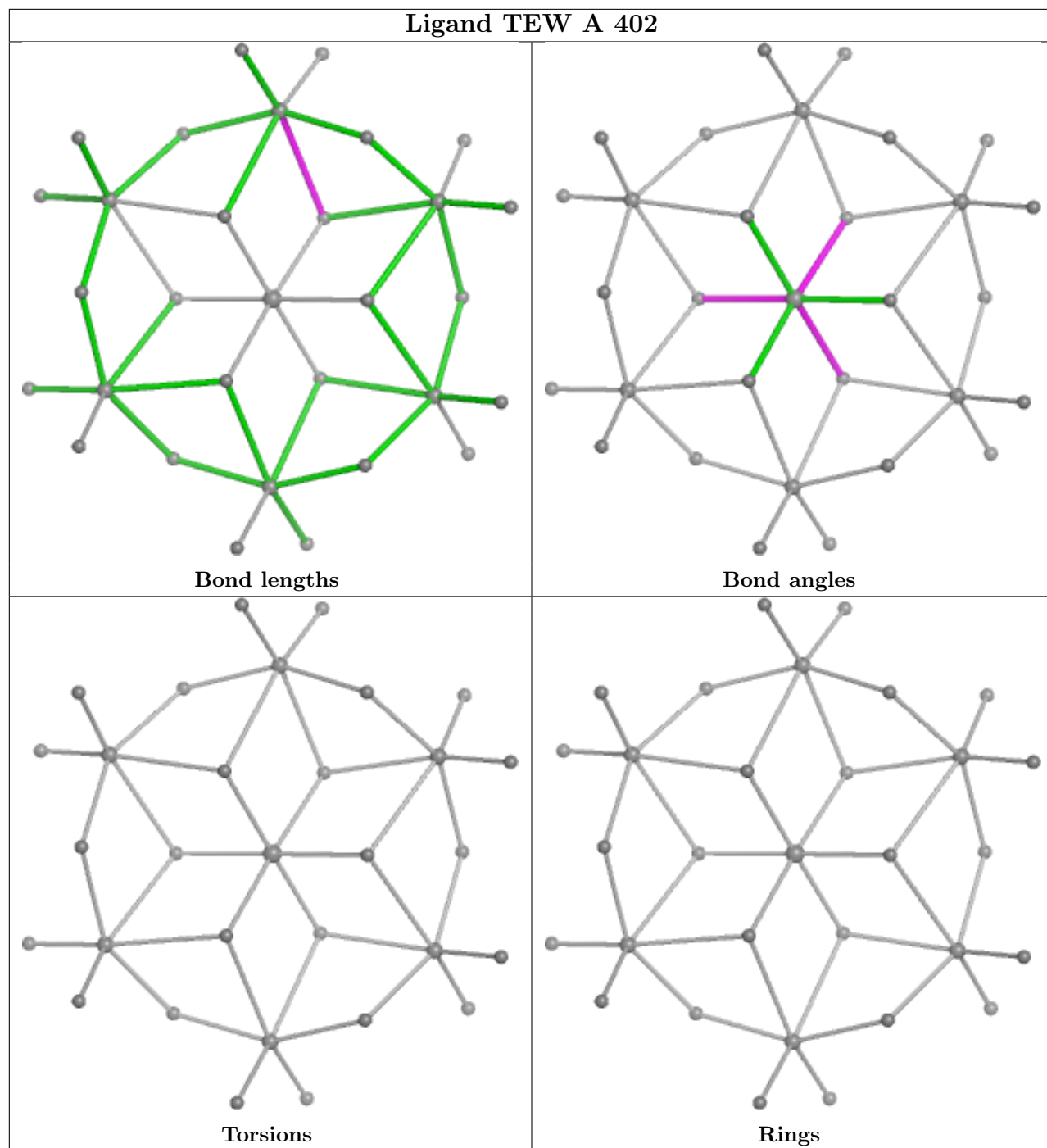
There are no ring outliers.

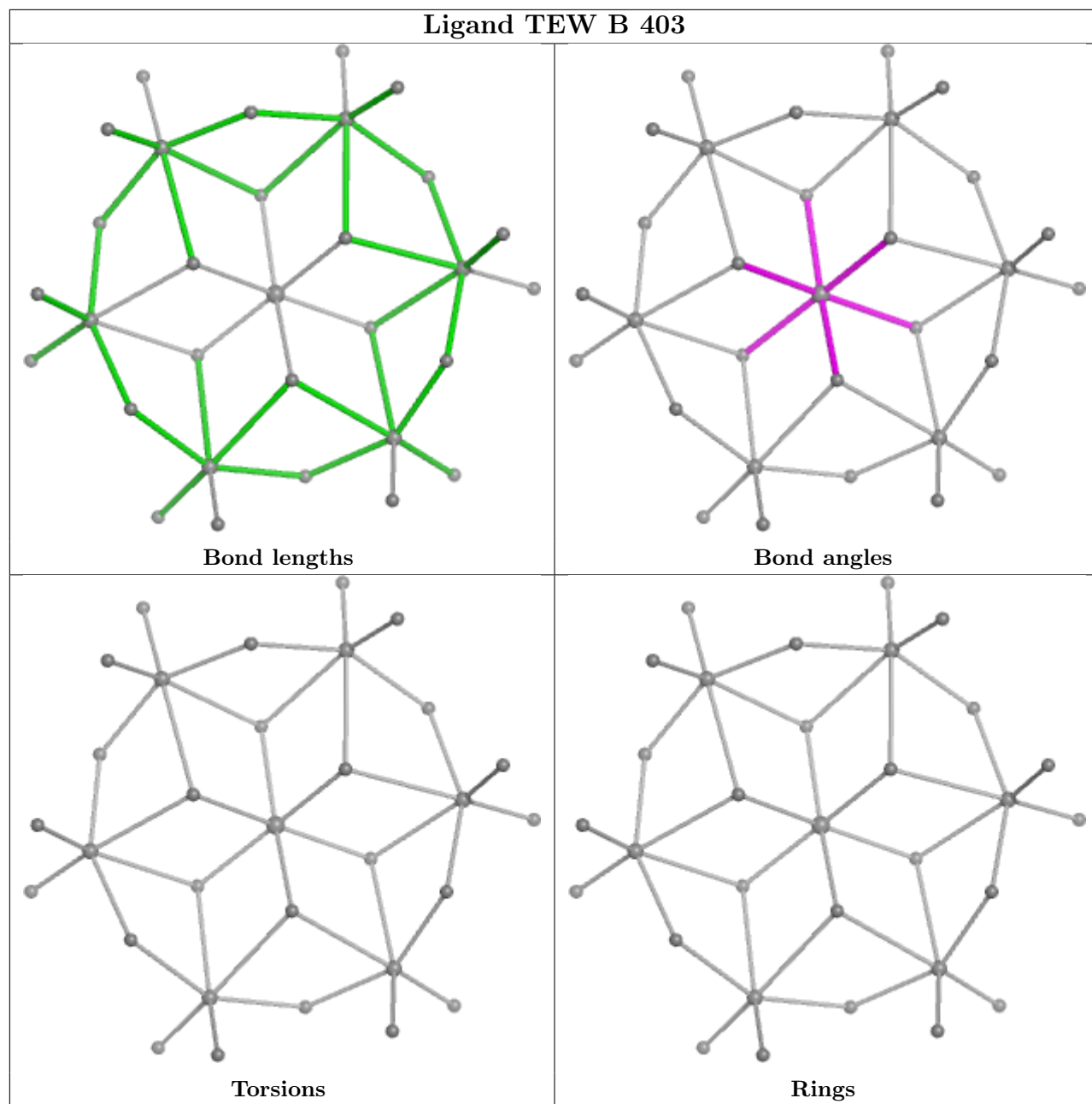
5 monomers are involved in 9 short contacts:

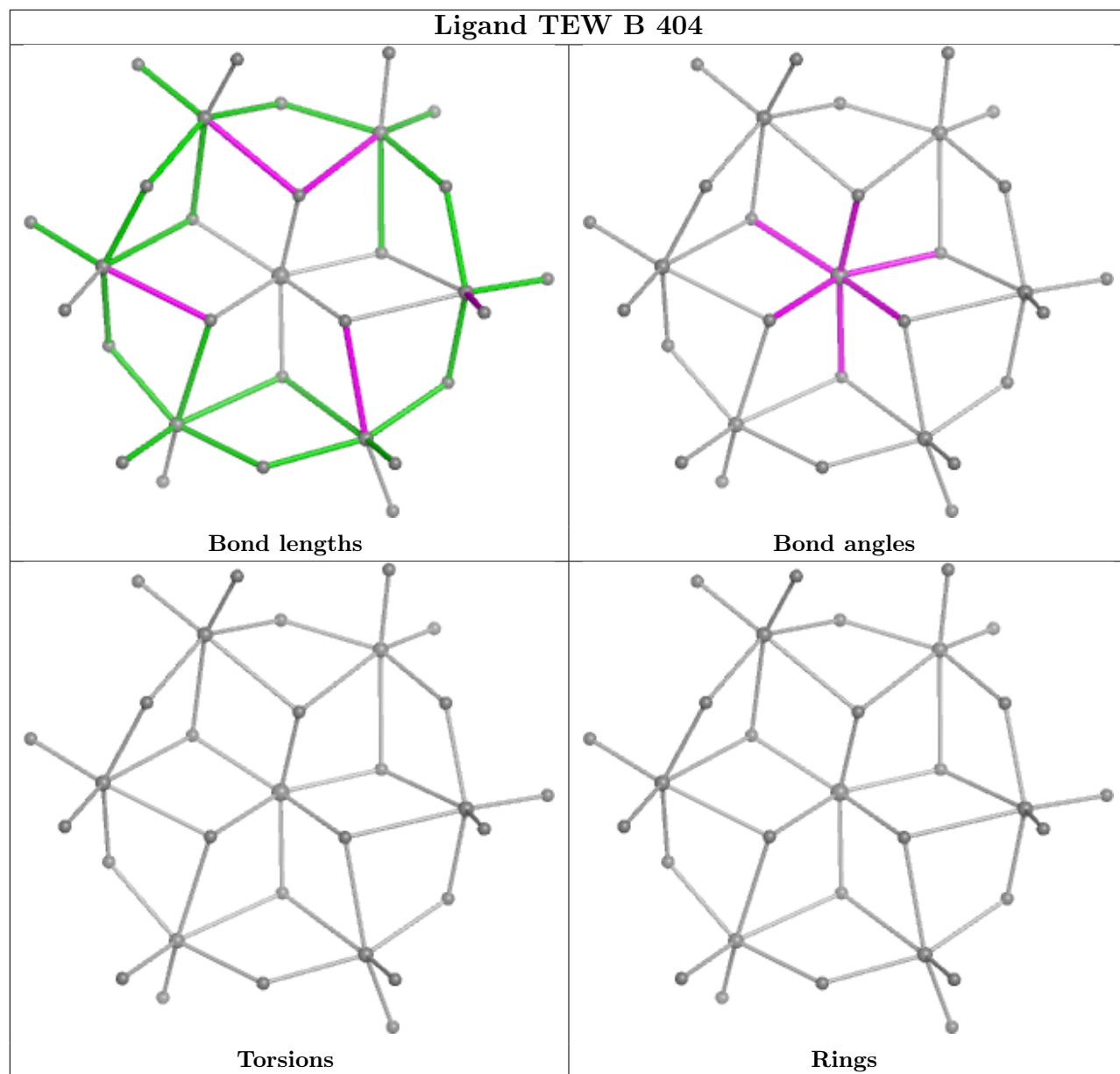
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	TEW	1	0
3	A	404	TEW	1	0
3	A	405	TEW	1	0
3	B	405[B]	TEW	4	0
3	B	405[A]	TEW	2	0

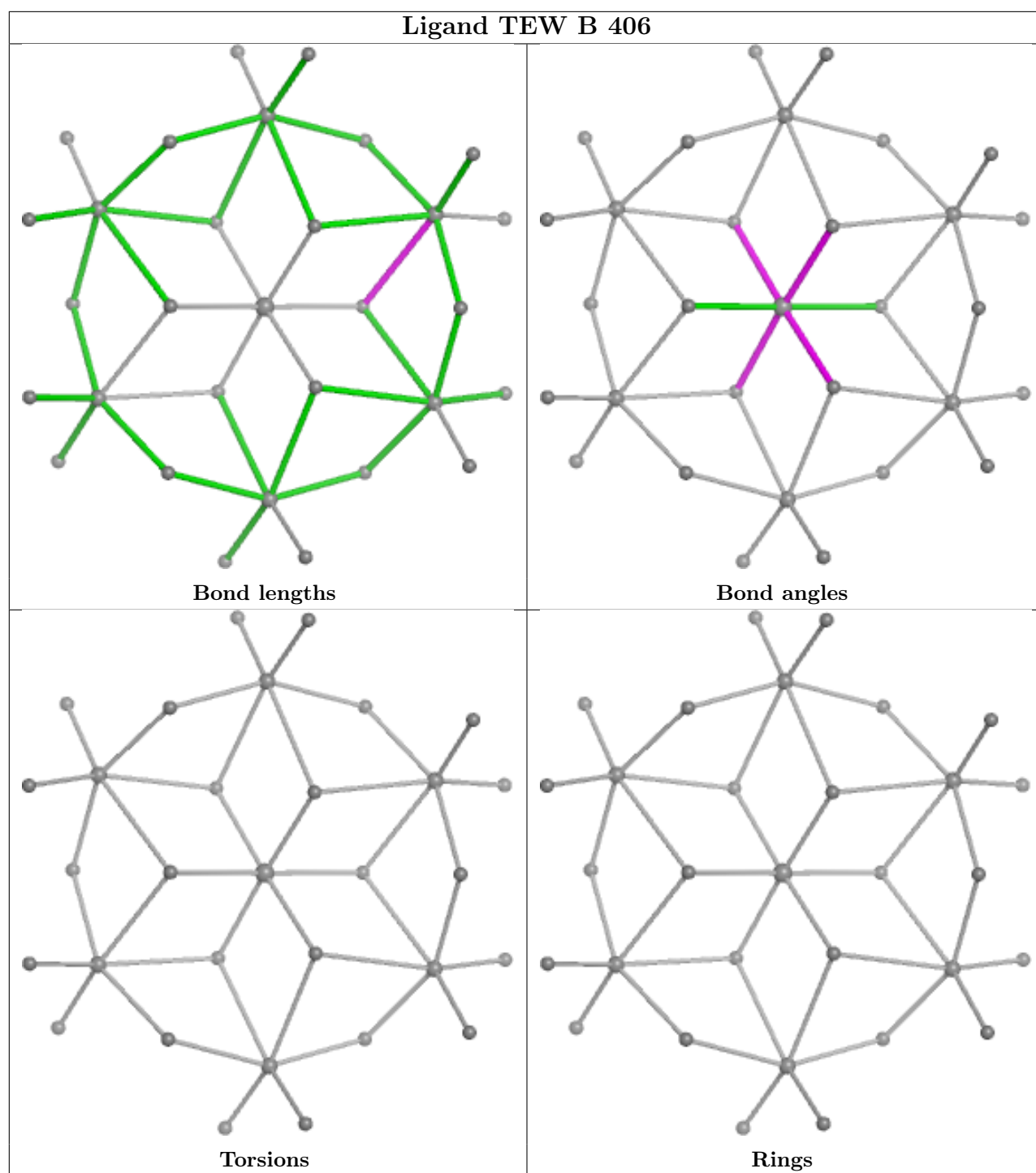
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



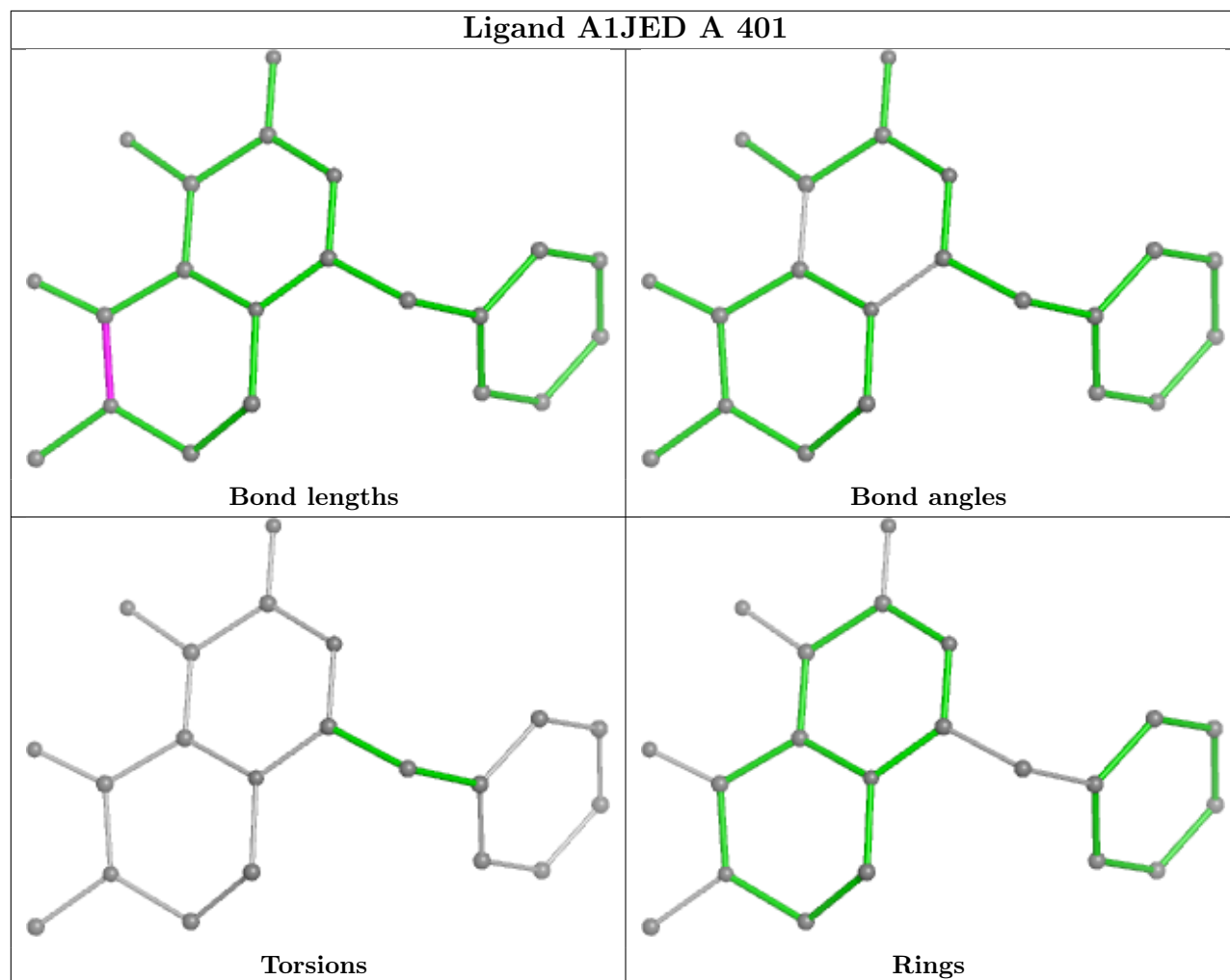


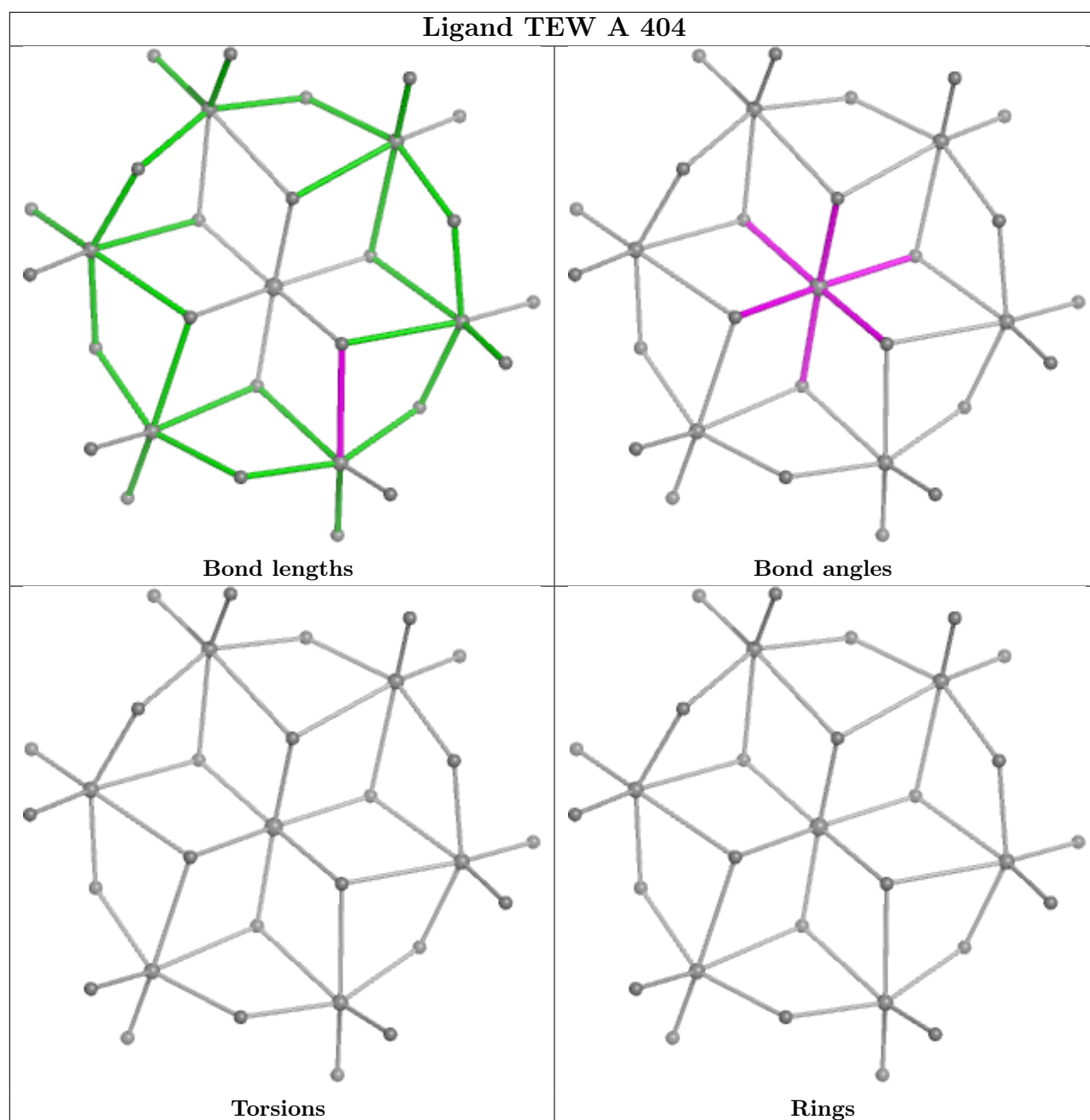




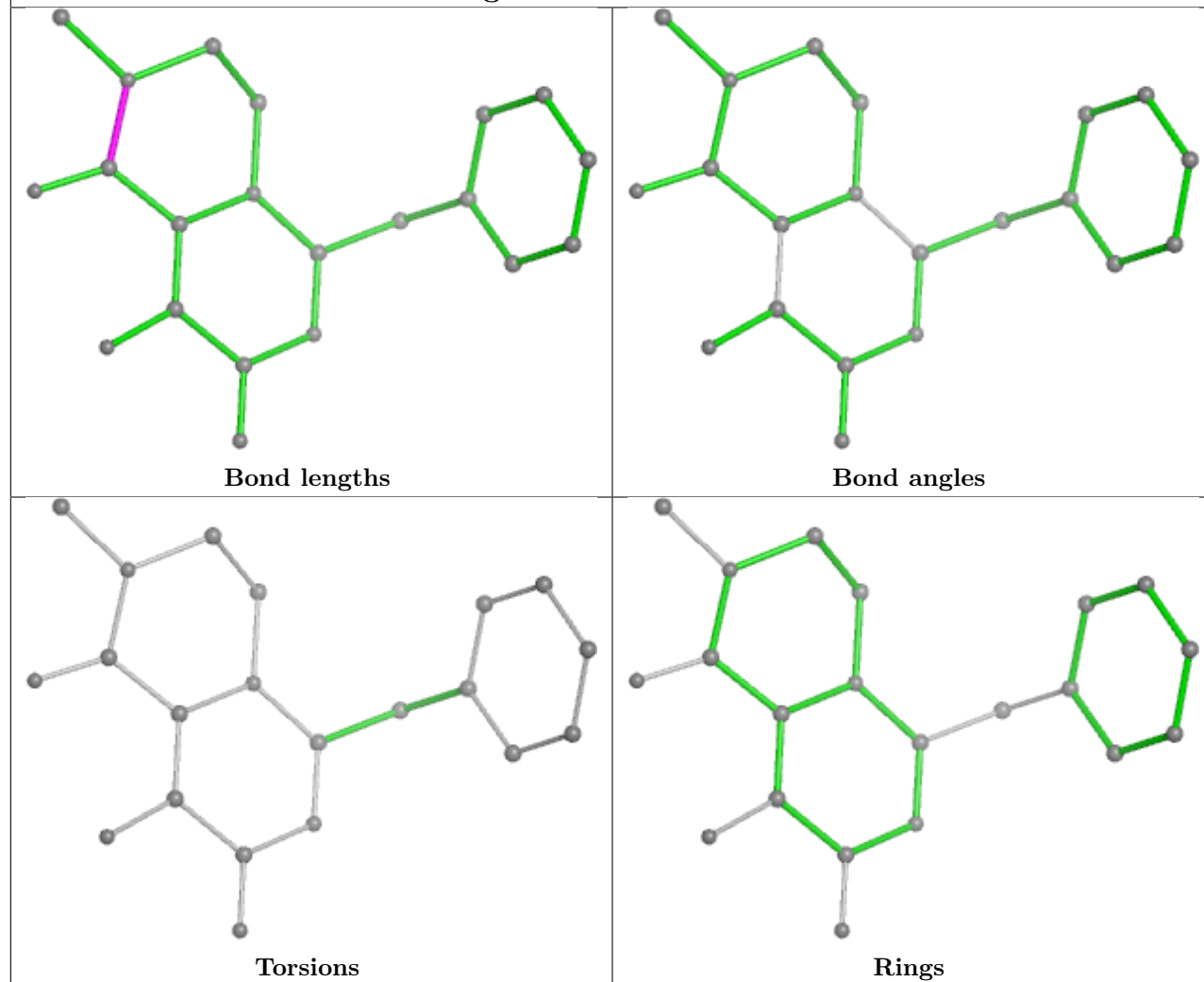


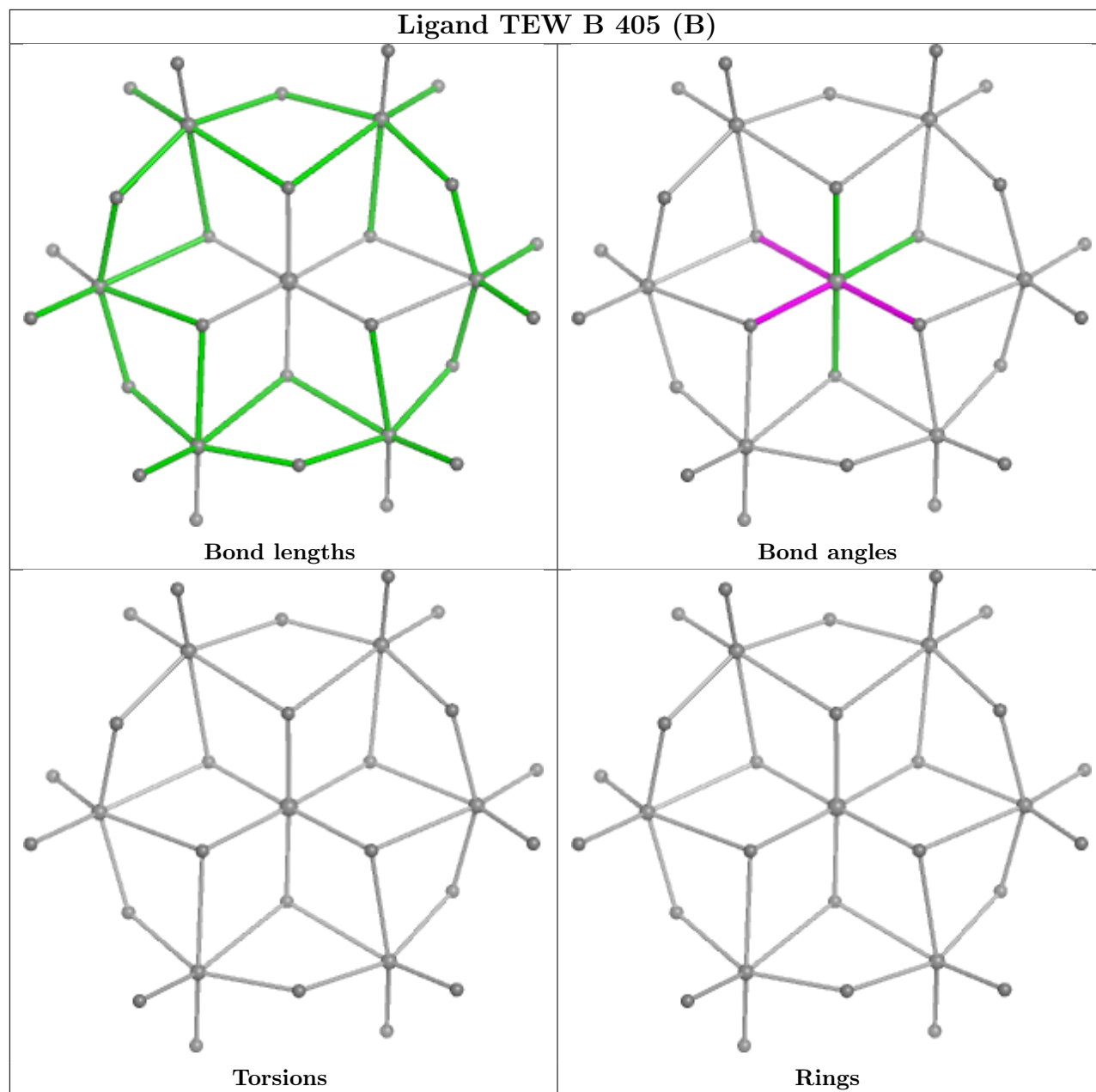
Ligand A1JED A 401



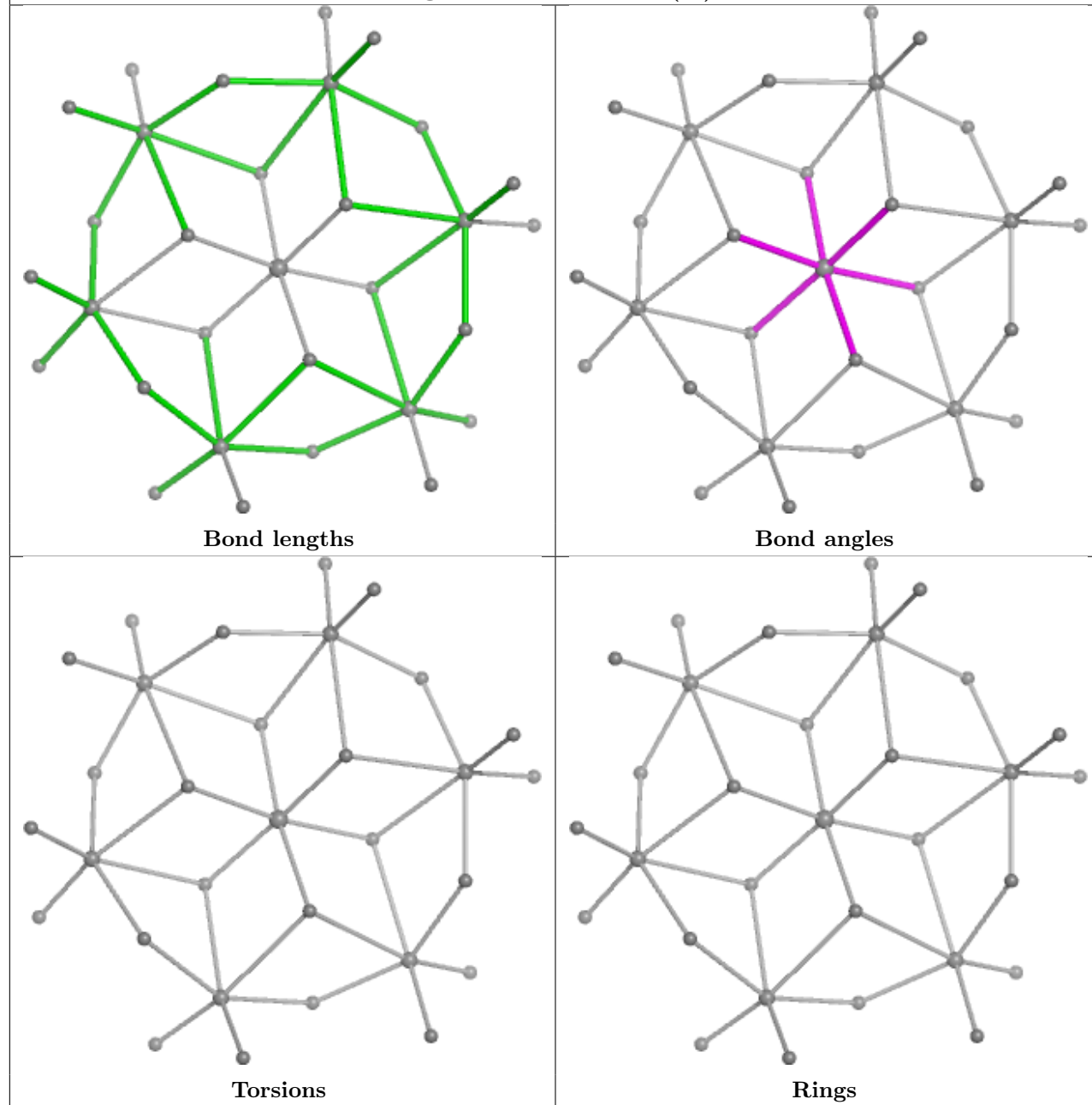


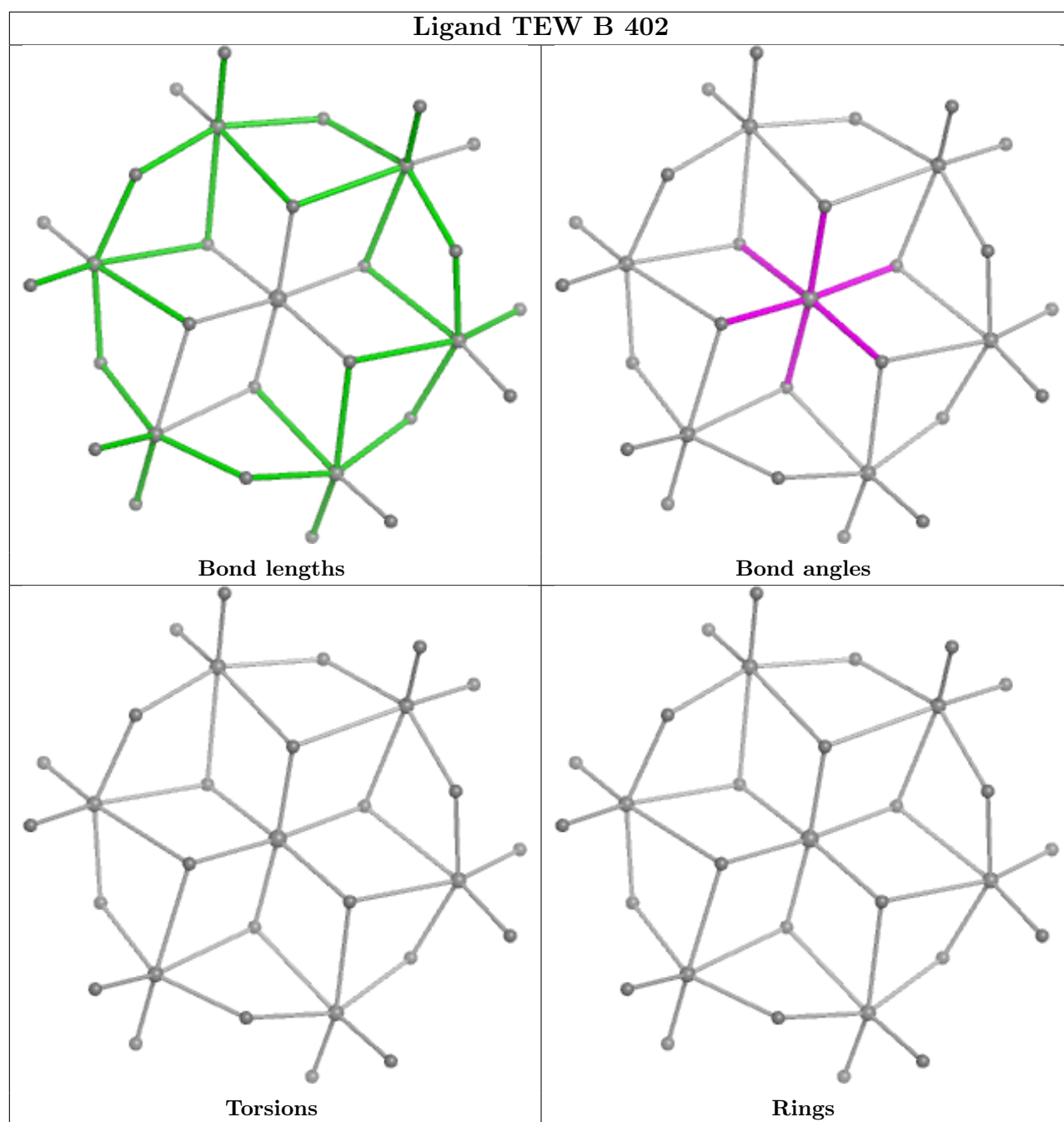
Ligand A1JED B 401





Ligand TEW B 405 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	308/342 (90%)	1.01	65 (21%) 3 3	13, 35, 68, 92	0
1	B	314/342 (91%)	1.04	69 (21%) 3 3	9, 32, 72, 85	0
All	All	622/684 (90%)	1.03	134 (21%) 3 3	9, 34, 71, 92	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	ALA	6.9
1	A	294	VAL	6.4
1	B	122	GLU	6.2
1	B	46	VAL	6.0
1	B	22	ASP	5.7
1	B	199	ALA	5.6
1	A	114	ALA	5.6
1	A	202	LEU	5.5
1	A	111	LEU	5.3
1	B	202	LEU	5.3
1	A	46	VAL	5.1
1	A	110	GLN	4.9
1	B	123	VAL	4.9
1	A	93	LYS	4.9
1	B	59	GLU	4.9
1	B	252	LYS	4.9
1	A	315	GLN	4.8
1	B	97	LEU	4.8
1	A	96	GLU	4.8
1	B	95	GLY	4.7
1	B	333	GLN	4.7
1	B	197	SER	4.5
1	B	23	ILE	4.5
1	A	107	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	121	GLN	4.5
1	A	268	TYR	4.3
1	B	200	LYS	4.3
1	A	126	PHE	4.3
1	A	109	LYS	4.2
1	B	109	LYS	4.1
1	B	125	LYS	4.1
1	A	123	VAL	4.0
1	B	268	TYR	4.0
1	A	105	ALA	4.0
1	B	124	GLU	4.0
1	B	111	LEU	4.0
1	A	312	GLY	3.9
1	A	97	LEU	3.8
1	A	265	PRO	3.8
1	A	267	LYS	3.7
1	A	325	VAL	3.7
1	A	263	LEU	3.7
1	A	94	SER	3.7
1	B	20	GLU	3.6
1	B	269	PRO	3.6
1	B	106	GLU	3.5
1	A	262	ARG	3.5
1	A	332	ARG	3.5
1	B	112	GLN	3.5
1	A	19	ARG	3.5
1	B	129	ARG	3.5
1	B	260	VAL	3.5
1	B	24	LYS	3.5
1	B	25	SER	3.4
1	B	198	GLU	3.3
1	B	13	VAL	3.3
1	A	264	ASP	3.2
1	A	258	GLU	3.2
1	B	110	GLN	3.2
1	A	59	GLU	3.2
1	A	13	VAL	3.1
1	A	266	ASN	3.1
1	B	270	VAL	3.1
1	B	108	GLU	3.1
1	B	313	GLU	3.1
1	B	107	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	323	SER	3.0
1	A	95	GLY	3.0
1	A	124	GLU	3.0
1	B	261	ARG	3.0
1	B	248	ASP	3.0
1	A	260	VAL	3.0
1	A	257	GLU	2.9
1	A	330	LYS	2.9
1	B	113	GLN	2.9
1	B	294	VAL	2.9
1	A	125	LYS	2.9
1	A	261	ARG	2.9
1	B	265	PRO	2.8
1	A	113	GLN	2.8
1	A	316	PHE	2.8
1	B	94	SER	2.8
1	B	263	LEU	2.8
1	B	262	ARG	2.8
1	A	108	GLU	2.8
1	A	112	GLN	2.8
1	B	4	GLN	2.8
1	B	332	ARG	2.7
1	A	319	GLU	2.7
1	A	272	GLU	2.7
1	A	106	GLU	2.6
1	B	201	LYS	2.6
1	B	203	PRO	2.6
1	B	259	ILE	2.6
1	B	98	ALA	2.5
1	B	308	LYS	2.5
1	B	126	PHE	2.5
1	B	295	GLU	2.5
1	A	129	ARG	2.5
1	A	320	ARG	2.5
1	B	21	ASN	2.5
1	B	96	GLU	2.4
1	B	275	LEU	2.4
1	A	333	GLN	2.4
1	A	181	ASP	2.4
1	B	241	ILE	2.4
1	A	4	GLN	2.4
1	A	292	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	236	GLU	2.3
1	B	92	LEU	2.3
1	A	304	GLU	2.3
1	A	99	LYS	2.3
1	B	257	GLU	2.3
1	B	330	LYS	2.3
1	A	295	GLU	2.3
1	A	239	ARG	2.3
1	A	60	THR	2.3
1	B	271	PRO	2.2
1	A	248	ASP	2.2
1	A	122	GLU	2.2
1	B	11	ALA	2.2
1	B	258	GLU	2.2
1	B	291	PRO	2.2
1	A	331	SER	2.2
1	B	285	GLU	2.1
1	B	12	ASP	2.1
1	A	269	PRO	2.1
1	A	221	GLU	2.1
1	A	135	LYS	2.1
1	A	12	ASP	2.1
1	A	45	ALA	2.1
1	A	293	SER	2.1
1	B	91	GLN	2.1
1	A	270	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

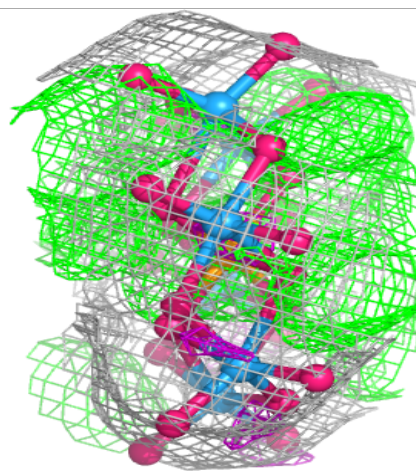
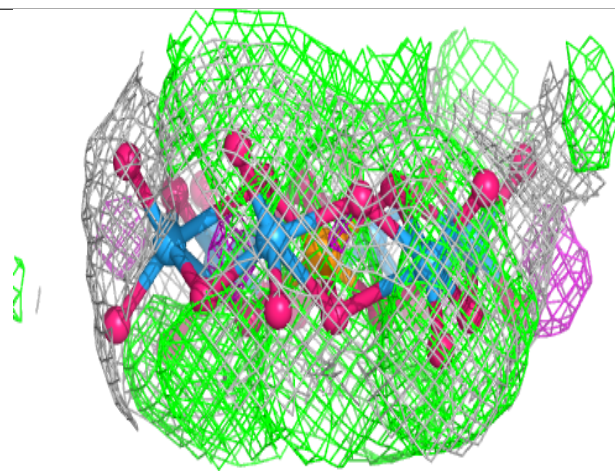
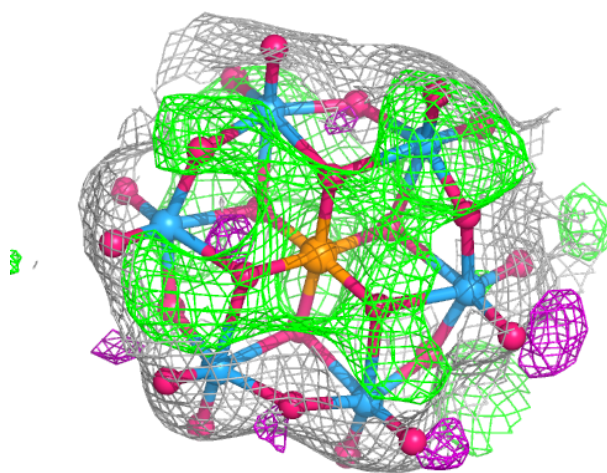
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TEW	A	405	31/31	0.85	0.20	124,125,126,126	31
3	TEW	B	402	31/31	0.87	0.23	79,82,86,87	31
3	TEW	B	405[A]	31/31	0.89	0.18	59,60,63,64	31
3	TEW	B	405[B]	31/31	0.89	0.18	50,54,56,56	31
4	MG	A	407	1/1	0.92	0.04	11,11,11,11	0
3	TEW	A	403	31/31	0.93	0.16	57,61,63,64	31
2	A1JED	B	401	21/21	0.94	0.08	15,17,21,21	15
3	TEW	A	402	31/31	0.94	0.15	51,52,55,56	31
2	A1JED	A	401	21/21	0.95	0.08	10,13,19,19	36
4	MG	B	408	1/1	0.95	0.05	15,15,15,15	0
4	MG	B	407	1/1	0.97	0.07	15,15,15,15	0
4	MG	A	406	1/1	0.98	0.06	11,11,11,11	0
3	TEW	B	404	31/31	0.99	0.06	25,31,37,38	0
3	TEW	B	406	31/31	0.99	0.07	48,51,56,57	0
3	TEW	A	404	31/31	1.00	0.04	18,21,23,23	0
3	TEW	B	403	31/31	1.00	0.04	18,20,23,23	31

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

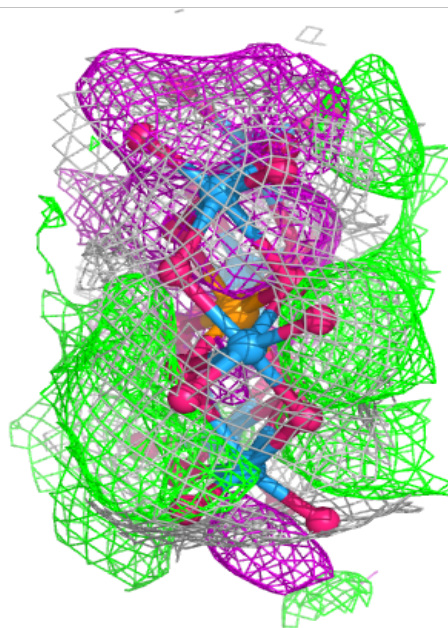
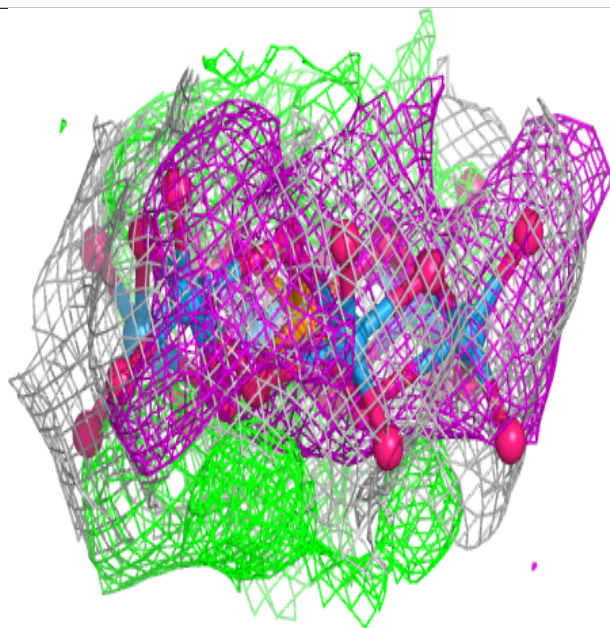
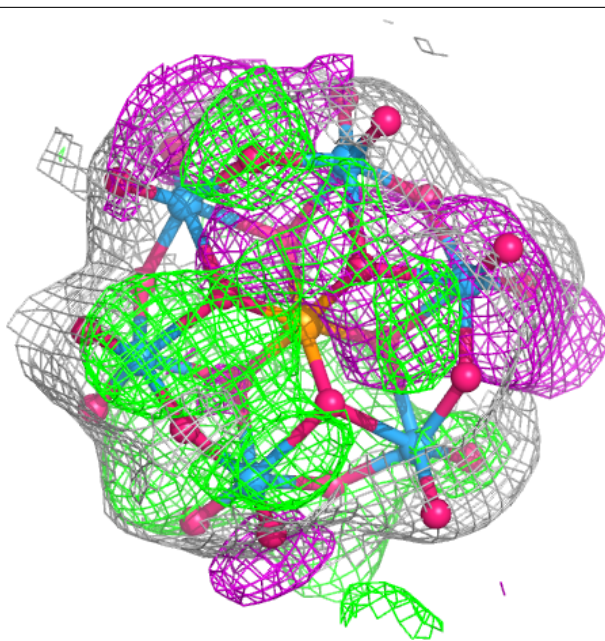
Electron density around TEW B 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



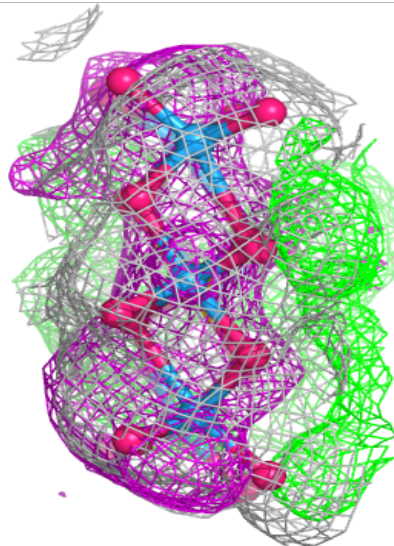
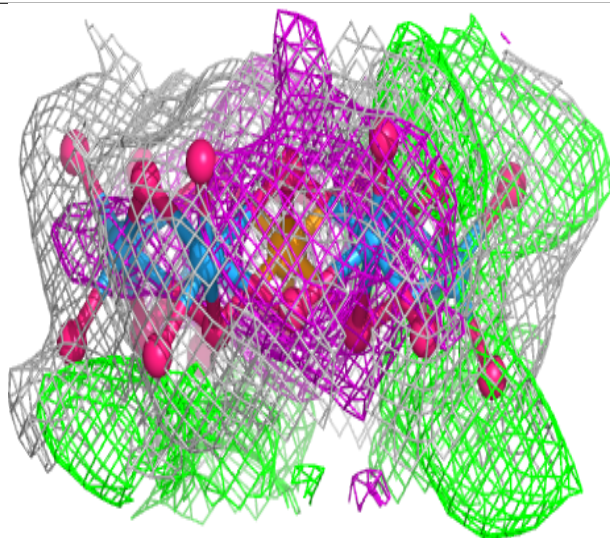
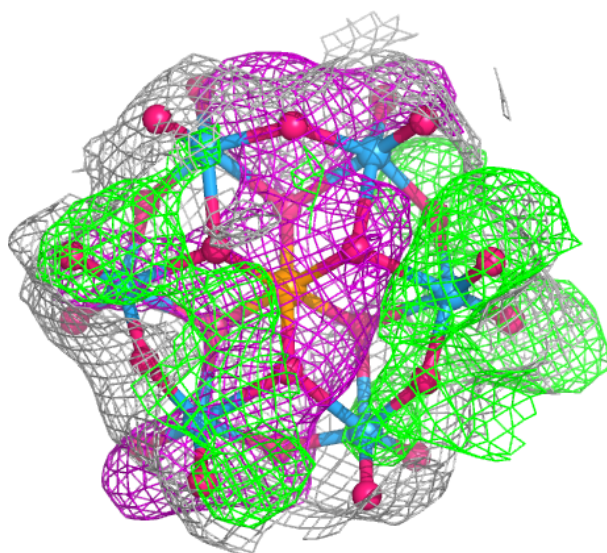
Electron density around TEW B 405 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



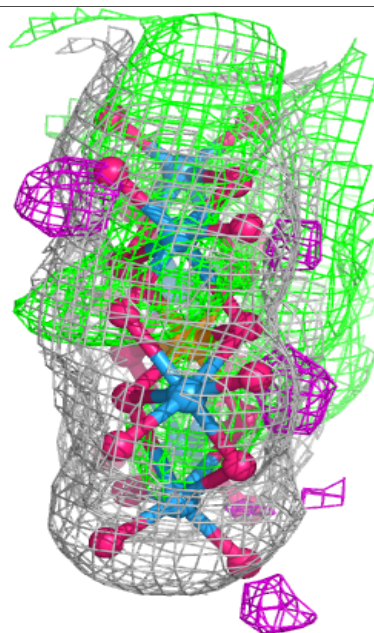
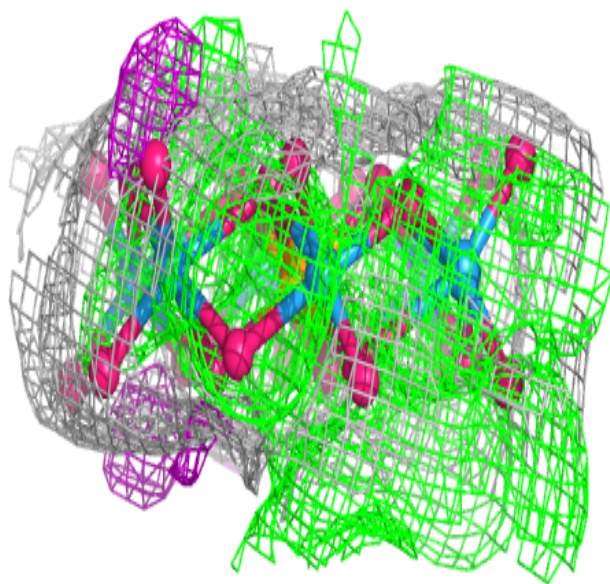
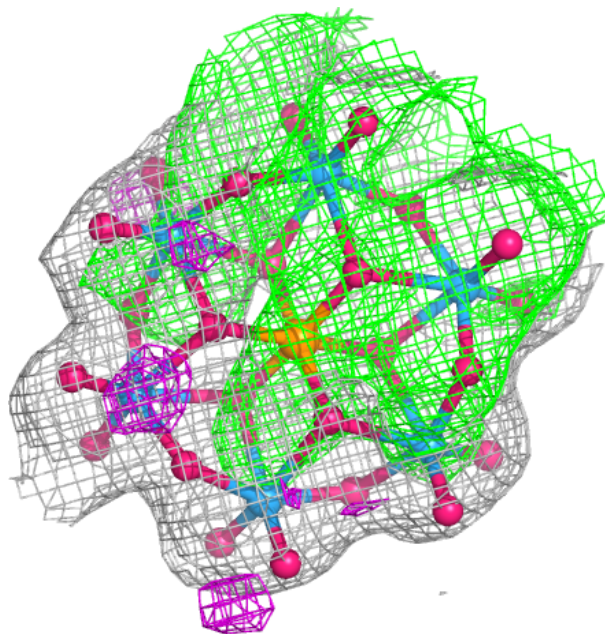
Electron density around TEW B 405 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



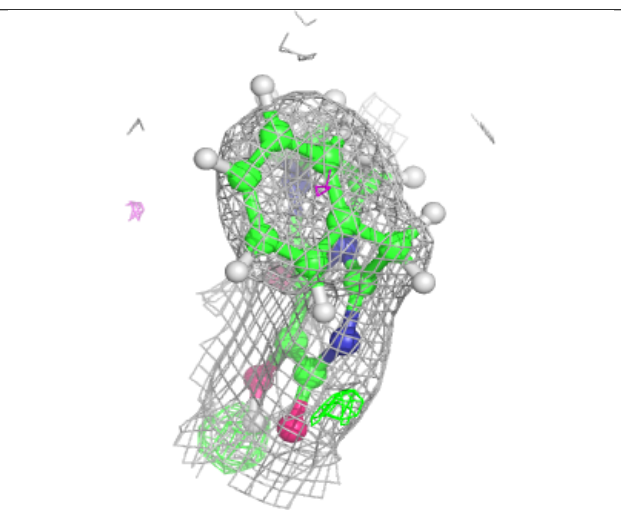
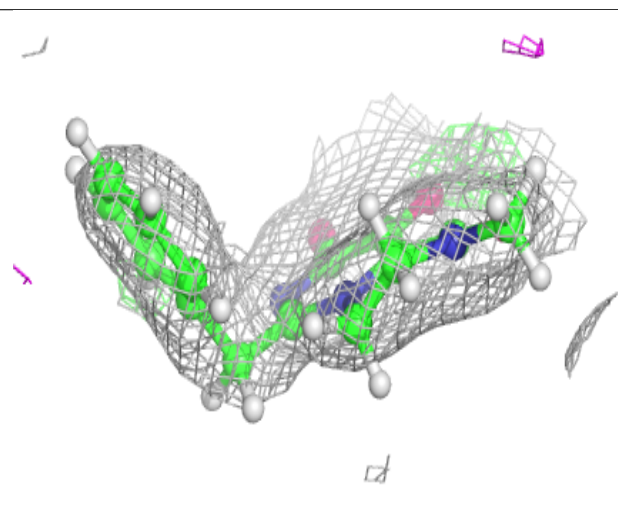
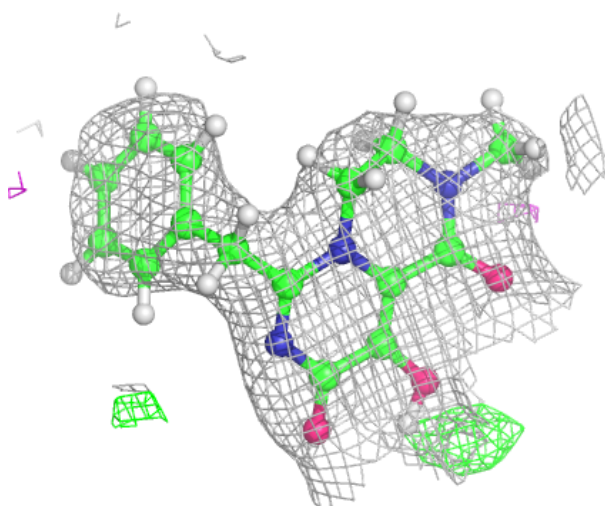
Electron density around TEW A 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



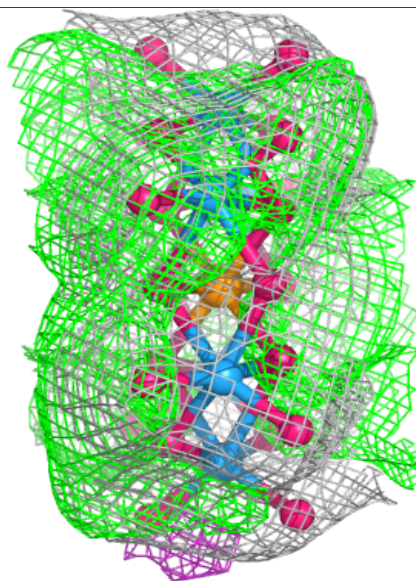
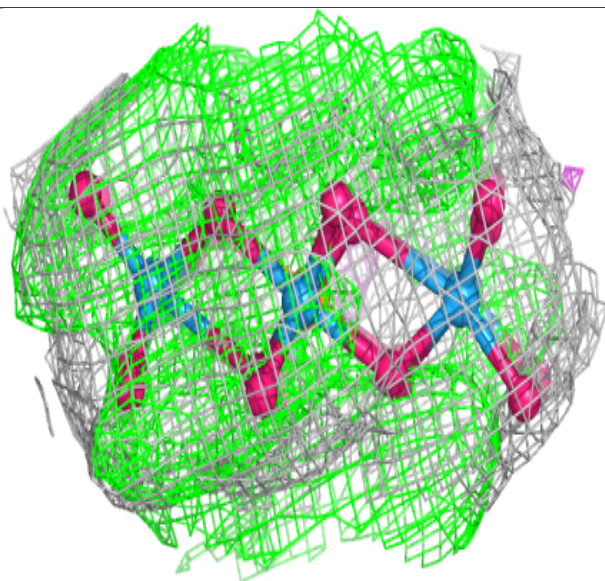
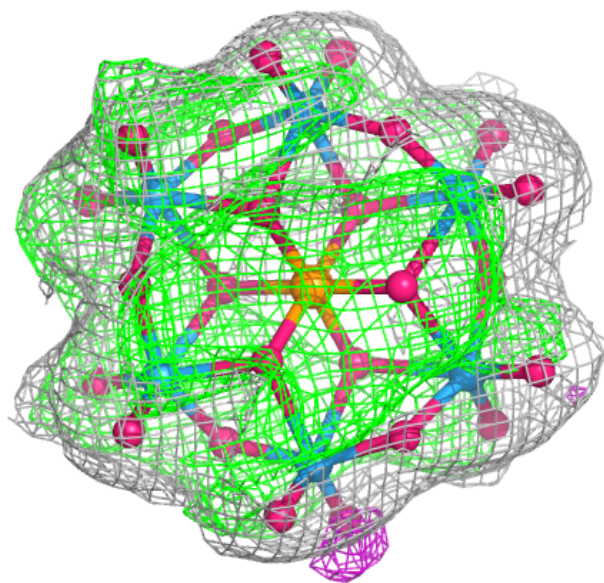
Electron density around A1JED B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



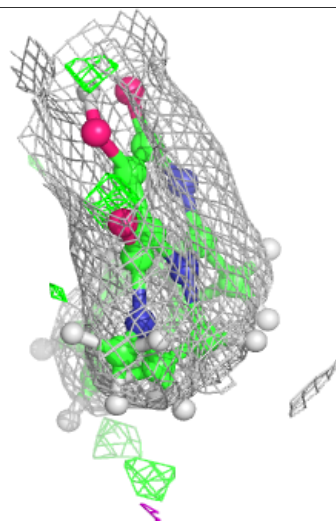
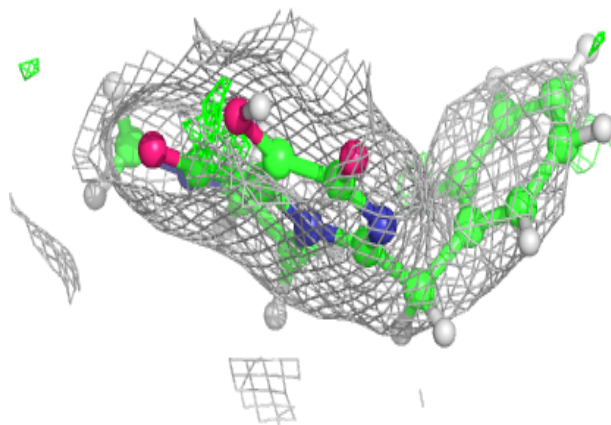
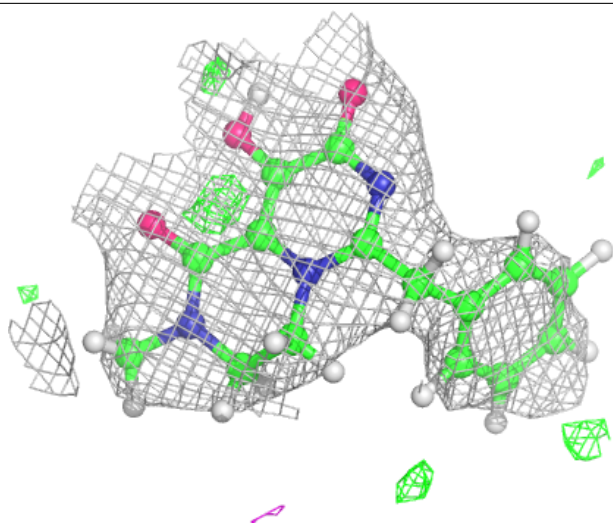
Electron density around TEW A 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



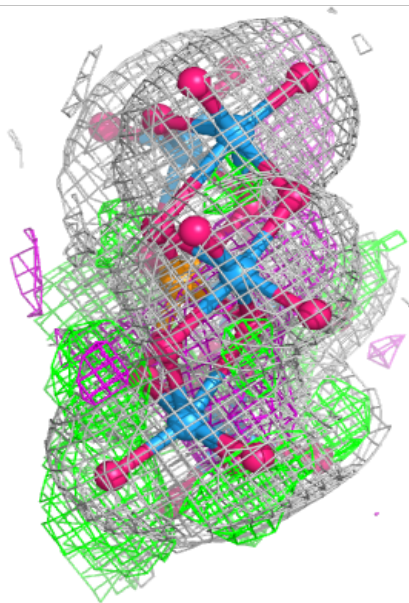
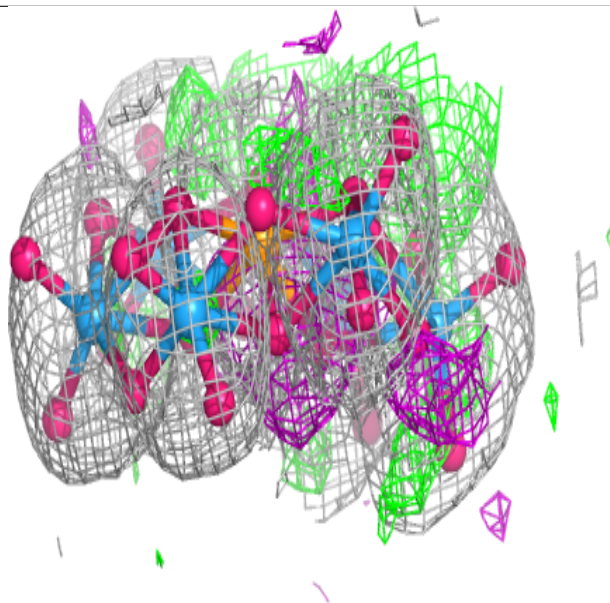
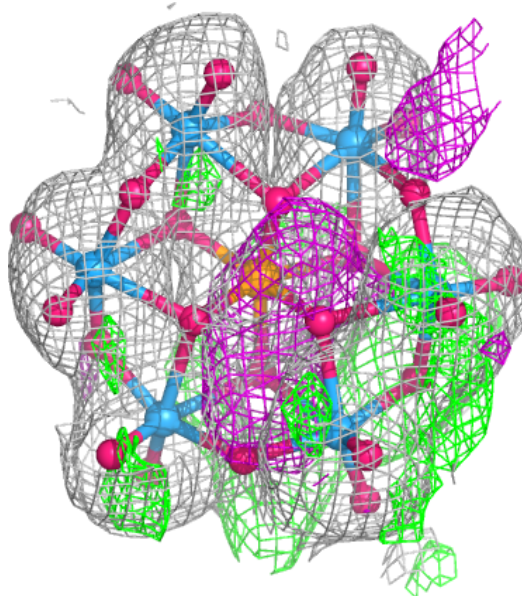
Electron density around A1JED A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



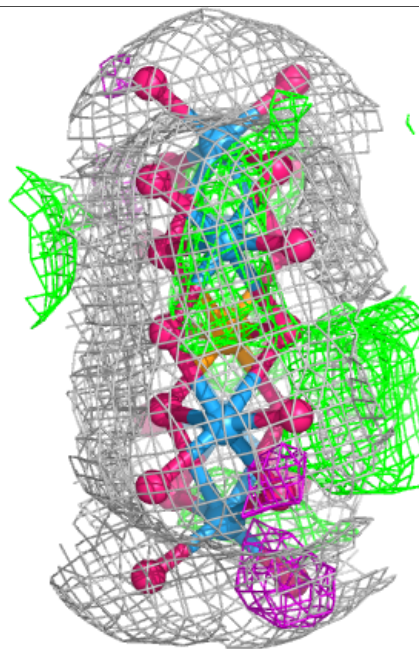
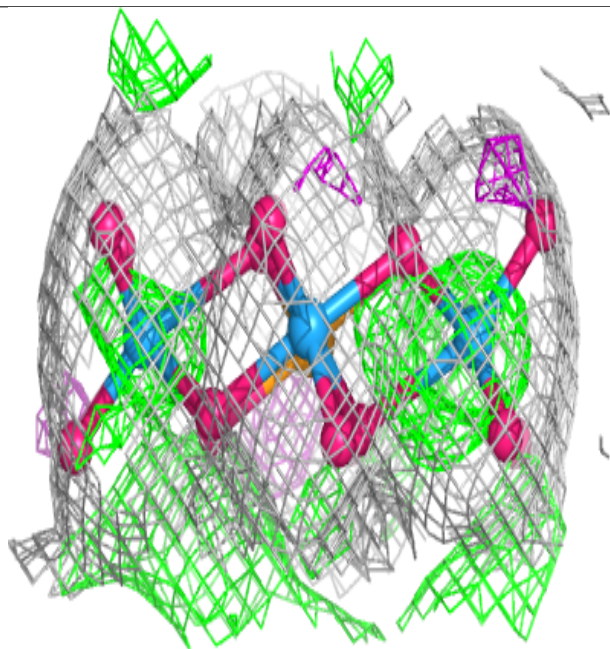
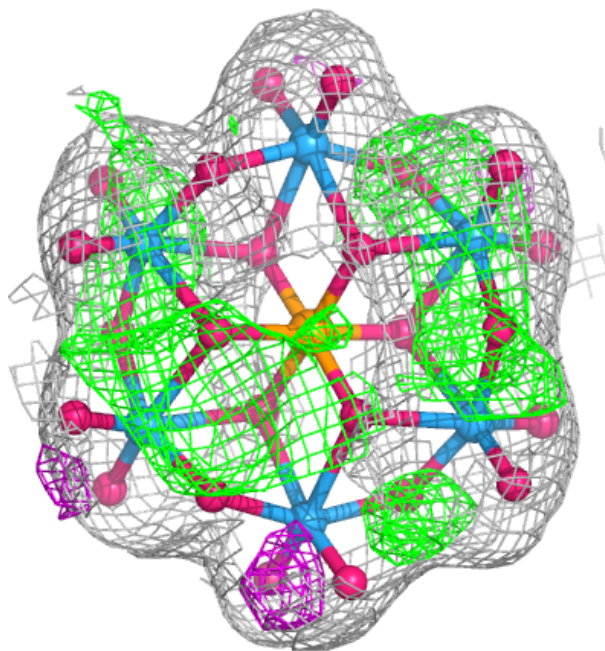
Electron density around TEW B 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



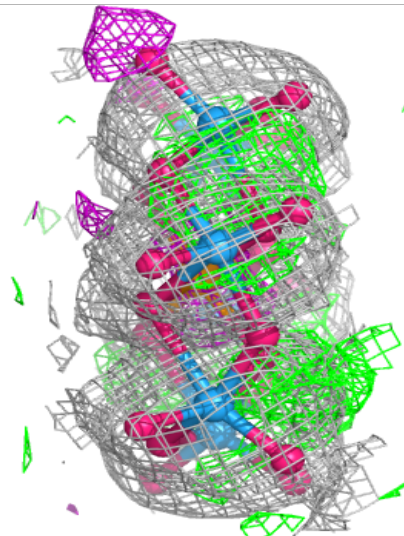
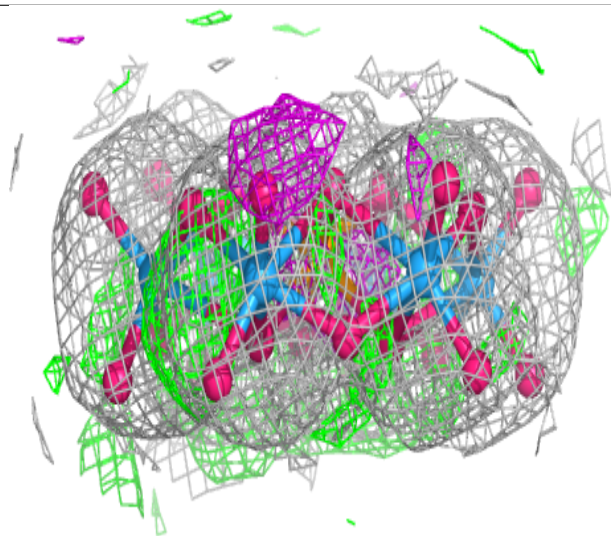
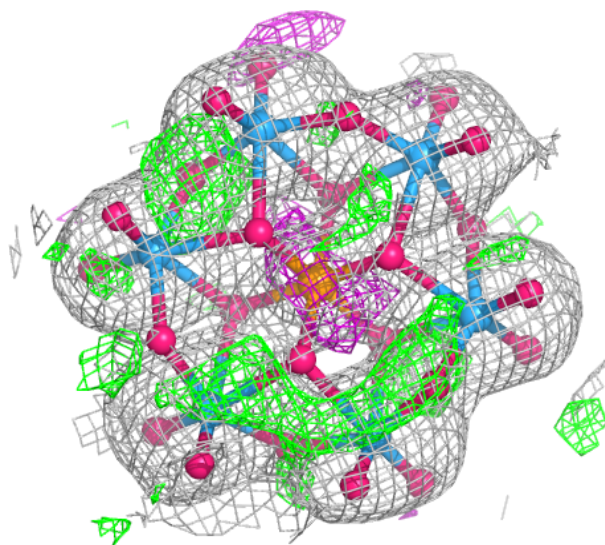
Electron density around TEW B 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



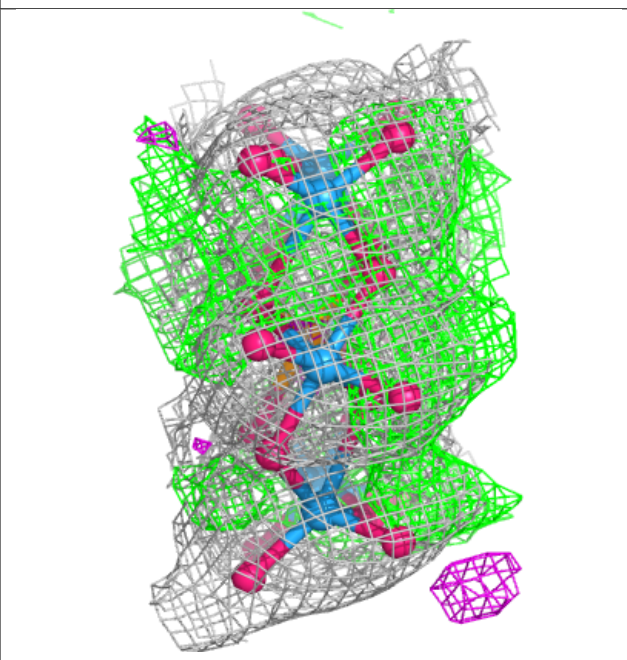
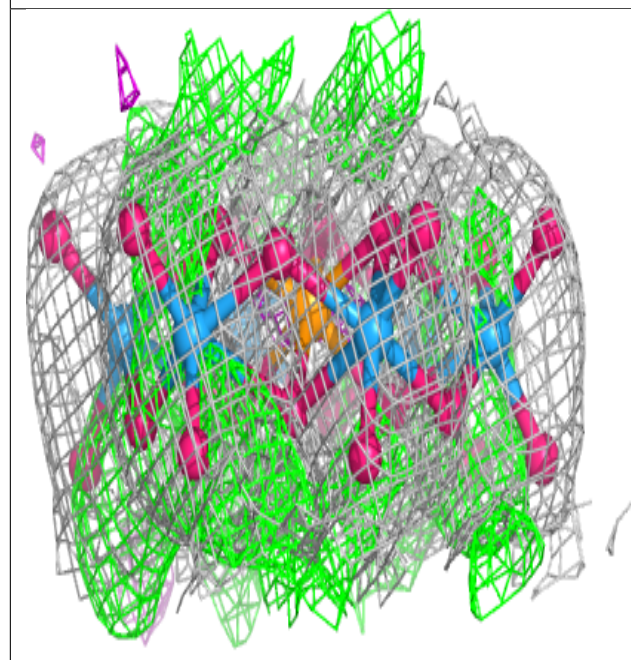
Electron density around TEW A 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TEW B 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.